A Synopsis

"Synthesis, Characterization and Application of $Cd_{1-x}Fe_xS$ thin Films"

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Format for submission of Ph.D. Synopsis /Work plan

Abstract of proposed work plan / Problem:

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1. Introduction:-

Thin films of transition metal chalcogenides have received much attention due to their wide range of applications in semiconducting devices, photovoltaic, optoelectronic devices, radiation detectors and solar energy converters [1–3]. Among them, cadmium Chalcogenides exert a pull on many researchers because they fulfill few of the requirements for several new electronic and optoelectronic devices such as light emitting diodes, photodiodes, blue green lasers etc., [4-5]. CdFeS is found to be a direct band gap semiconductor which makes them interesting for Photoelectrochemical solar cells. The process of doping transition metals with CdS which has been found numerous applications in the region of visible. Measurement of magnetic properties at room temperature for Fe doped nanocrystals (CdS:Fe) was analyzed by Murali et al. [6]. Quenching effect of photo- conductivity on Fe doped CdS (CdS:Fe) thin films prepared using spray pyrolysis was reported by Badera et al. [7]. To the best of our knowledge, no such report that have been focused the Fe doped CdS thin films (CdS: Fe) using a cost effective chemical technique for Photoelectrochemical properties.

Preparation of good quality $Cd_{1-x}Fe_xS$ thin films

It is proposed to synthesize $Cd_{1-x}Fe_xS$ thin films by chemical methods (chemical bath deposition / spray Pyrolysis). Initially the good quality $Cd_{1-x}Fe_xS$ thin films will be deposited on glass and conducting glass substrates. The various preparative parameters like concentration of the ingredients, deposition temperature, thickness and other parameters will be optimized to get good quality $Cd_{1-x}Fe_xS$ thin films. The as deposited

thin films will be characterized by various characterization techniques in the following manner.

[A] Structural Analysis:

An X-ray diffraction technique will be employed to know the structural changes as a result of Fe incorporation into CdS. The interplanar distance (d), intensities of reflections, lattice constants and crystal dimension will be examined and their dependence on composition will be studied.

[B] Compositional Analysis:

The compositional analysis will be done by means of an EDAX or EDS technique and correlation will be made with as taken and observed contents of Cd^{2+}, Fe^{2+}, S^{2-} elements.

[C] Microscopic Studies:

To study the surface morphological features SEM/TEM technique will be utilized. The crystallographic and morphological information will be used to explain the transport mechanism and optical properties.

[D] Optical Properties:

The optical constants as optical absorption coefficient (α), the energy band gap (E_g) and mode of optical transition will be determined from optical studies. For this purpose optical absorption / transmission / reflection spectra of the as deposited $Cd_{1-x}Fe_xS$ series will be studied.

[E] Electrical transport properties:

The electrical conductivity and thermo-electric power will be measured of all these as deposited thin films. Various terms like carrier concentration (n), mobility (μ), activation energy (E_a) and barrier height ($\square_B$) will be determined.

[F] Photoelectrochemical studies:

Photoelectrochemical studies will be under taken by forming a cell composed of these as deposited film electrode as active photo electrode and a suitable electrolyte. The various cell characteristics under dark and under illumination will be studied to examine the various cell parameters such as short circuit current (I_{sc}), open circuit voltage (V_{oc}), series resistance (R_s), shunt resistance (R_{sh}) flat band potential (V_{fb}) and power output will be determined. An optimum composition yielding better performance will be searched out and its correlation with observed film properties will be studied.

[G] Effect of technical parameter:

To boost the cell performance effect of technical parameter such as material thickness / heat treatment / impurity concentration will be undertaken.

2. Review of Literature and Development in the subject

In recent years, considerable interest has been shown in the synthesis and Photoelectrochemical properties of semiconductor thin films. CdS belongs to the II–VI group and is n-type in nature [8]. Electron–hole pairs generated in CdS are well separated with electrons being highly localized [9-10]. So it is the most studied nanocrystalline semiconductor as a photo anode in Photoelectrochemical (PEC) solar cells because of its suitable band gap, long lifetimes, and important optical properties, excellent stability, easy fabrication and numerous device applications. The significant properties (electrical, optical and magnetic) are strongly modified by the doping of Mn^{2+}, Fe^{2+} and recently Co^{2+} [11-12] because of the sp–d exchange interaction between the localized d electrons of the transition metal magnetic ions and the mobile carriers in the conduction or valence band. In contrast with Mn^{2+}, Fe^{2+} possesses not only both spin and orbital moment (S = 2, L = 2) as well one more electron, so Fe $3d^{6+}$ state is located above the Mn $3d^{5+}$ state in a semiconductor band structure. Therefore, the nanocrystals containing substitutional Fe^{2+} ions have been studied recently, because of their interesting electrical, optical and magnetic properties [13-14].

A number of techniques that have been reported to prepare CdS thin films such as thermal evaporation [14-15], electron beam evaporation [16], vacuum evaporations [17], RF sputtering [18], pulsed laser deposition [19], chemical bath deposition [20] etc.

3. Objectives of Research/Proposed Hypothesis

Following are the objectives of our research work

1. To deposit good quality $Cd_{1-x}Fe_xS$ (x = 0 to 1) thin films by chemical route.
2. To study various properties such as thickness, optical, electrical properties of as deposited samples.
3. To study micro-structural and morphological features of as grown $Cd_{1-x}Fe_xS$ thin films.
4. To use these films in Photoelectrochemical solar cells and study their characteristics.
5. To study the effect of technical parameter on solar cell performance of optimum samples of $Cd_{1-x}Fe_xS$.

4. Methodology to be adopted:

The chemical method will be used to synthesize the $Cd_{1-x}Fe_xS$ thin films. Unlike the physical methods of preparation of thin films involving evaporation or ejection of material from a source, chemical methods of thin film deposition entail a definite chemical reaction. The chemical method is presently attracting considerable attention as it does not require sophisticated instrumentation like vacuum system and other expensive equipments. The starting chemicals are commonly available and cheap. The preparative parameters are easily controllable and better orientations and improved grain structure can be obtained.

In our present work, $Cd_{1-x}Fe_xS$ thin films will be prepared by a chemical method. The deposited thin films will be characterized to study the structural, morphological, optical and electrical properties by means of XRD, SEM, UV-Vis spectrophotometer respectively. The Photoelectrochemical solar cell properties of $Cd_{1-x}Fe_xS$ thin films will be studied.

5. Importance of study / Society applications:

Recently, II–VI group binary semiconductors have received much attention due to its wide range of applications in fabrication of so many solid state devices such as solar cells, opto-electronic devices and solar selective coatings. Among them, CdS is found to be an excellent material with a band gap value around 2.5eV which make them interesting for the fabrication of Photoelectrochemical solar cells, because of its compatibility of band gap with solar spectrum. CdS thin films are normally crystallized in hexagonal (wurtzite) structure

Diluted magnetic semiconductors (DMSs) [21] have attracted much attention due to the wealth of scientific information and potential technological applications. DMSs are semiconductor alloys formed by randomly replacing a fraction of the cations with magnetic ions, e.g., Fe^{2+} in CdS to form $Cd_{1-x}Fe_xS$. In these materials, the large sp–d exchange interaction between magnetic ions and electrons in valence band [22–24] can lead to a number of unusual electronic, optical and photo properties.

Another important advantage of using these materials in their binary and ternary forms is that they are capable of being formed as this film by various methods and at low cost. This material, in its thin film form has received a considerable attention in optoelectronic device and solar cell. The Photoelectrochemical cells are one of the most promising semiconductor/ liquid junction solar cells. As solar energy is one of the promising energy sources for the future, a large number of researchers have concentrated on this aspect and a keen attention is required in this regard. A variety of electrochemical photovoltaic cells have been fabricated and investigated to convert the solar energy into electrical energy.

Potentially, there are several advantages of PEC cells for solar energy conversion over conventional PV devices or Schottky barrier solar cells [12,13]: (1) PEC devices can store energy in the form of conventional fuel and can convert light to electrical energy as well; (2) PEC devices can be fabricated and modified with considerable ease. Contrary to PV devices, no solid–solid junctions are demanded in PEC. The band bending characteristics of the semiconductor can be conveniently varied by suitable

choice of electrolyte and cell variables; and (3) PEC cells do not have problems associated with different thermal expansions of solid–solid junction [25].

6. Proposed work Plan / Formulation and Structure of Study:

Year-wise plan of work and targets to be achieved

Year I-Plan:

In the first year of the research literature survey and data collection will be done in order to get more information about work already done and scope of the present work. The literature survey includes collection of Journals, books, and related research papers. The chemicals of high purity will be purchased and efforts will be made to deposit good quality $Cd_{1-x}Fe_xS$ thin films. At the end of the year two progress reports will be submitted.

Year II-Plan:

In second year, all preparative parameters will be optimized in order to get good quality thin films of $Cd_{1-x}Fe_xS$ on non-conducting and conducting glass substrates. The as deposited films will be characterized by various characterizing techniques such as X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Analysis by X-ray (EDAX), UV-Vis photo spectrometer and photo electrochemical solar cell study. The results will be analyzed and efforts will be made to publish two or more research papers in reputed research journals. Two progress reports will be submitted at the end of this year.

Year III-Plan:

In the last year, an optimum composition yielding better result will be searched out and effect of technical parameter such as material thickness / heat treatment / impurity concentration will be studied. The results obtained will be analyzed and an attempt will be made to publish it in the reputed journals. Also efforts will be made to

share results in the national and international Seminars, Conferences and Workshops etc. during this year. At the end of the year other progress reports will be submitted.

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